

Remarks

This response is being submitted within one month after the shortened statutory period set for responding to the Office Action that was mailed on May 8, 2003. Therefore we are enclosing herewith a petition and the fee for an extension of time.

Hereinafter the Claims that are pending prior to the entry of the amendments in this response are called currently pending Claims. This response does amends Claim 18. The above-identified US patent application has 5 independent Claims [currently pending Claims 1, 13, 33 and 44 and amended Claim 18] and a total of 57 Claims [currently pending Claims 1, 3-17, 19-44 and 46-59 and amended Claim 18]. The Examiner states on the bottom of page 7 that Claim 18 contains the expression "comparing" and interprets it as comprising". Applicants agree with the Examiner and amended Claim 18 accordingly. Applicants have previously paid for 59 total Claims and 5 independent Claims. Therefore, no excess Claims fee has to be paid with this response.

I. Claim Rejections – 35 USC § 102

The Examiner rejects Claim 1 under 35 U.S.C. 102(e) as being anticipated by US Patent No. 5,666,217 of Kaneko *et al*, hereinafter called US '217. Applicants respectfully traverse the Examiners assertion.

1. The Claim limitations of currently pending Claim 1 are as follows:

A liquid crystal device comprising:
a layer of a liquid crystal material contained between two spaced cell wall carrying electrodes structures and an alignment treatment on at least one wall,
characterized by
means for reducing anchoring energy at the surface alignment on one or both cell walls, comprising:
an oligomer or polymer within the liquid crystal material at the cell walls.

2. The claimed device is characterized by means comprising an oligomer or polymer for reducing anchoring energy at the surface alignment on one or both cell walls. Thus there is an alignment treatment on at least one wall, and means for reducing anchoring energy at that surface alignment, comprising an oligomer or polymer within the liquid crystal material at the cell walls.
3. The Examiner interprets the recitation "within the liquid crystal material at the cell walls" to mean that the liquid crystal is surrounded by a polymer-containing material that reduces anchoring energy (surface potential)" in paragraph 2 on page 3. The Applicants traverse the Examiner's interpretation. The Examiner equates anchoring energy with surface potential. It is inadmissible to do so without complying with Rule 104(d)(2) and the examiner is requested to supply the affidavit required by the rule or to cite a prior art document supporting this interpretation. As discussed at page 12, lines 1-3 of the instant Application anchoring energy arises from surface topography features such as grooves or gratings and from chemical bonding interactions. Therefore, the anchoring energy is reduced for example by changing the chemical bonding.

Surface potential is a measurable voltage. It is defined in US '217 at column 7, lines 56-61, and further description gives a method of measuring surface potential (or potential difference). Thus, anchoring energy and surface potential are not exactly the same thing. If the Examiner believes that they are exactly the same thing, please provide a prior art document supporting that position or the affidavit required by Rule 104(d)(2). In this connection, please review the article by Andrienko & Allen enclosed herewith.

More importantly, the word "surround" is not the same thing as "within" - the term used in the claims. With all due respect to the Examiner, taking artistic license with the wording of the claims and fashioning a prior art rejection based on such a re-worded version of the claims may make the Examiner's rejection seem more palatable, but the Applicant will certainly object (and does object) to that sort of Examination practice. In the future, the Examiner is respectfully requested to confine his analysis to

the specific language of the claims.

4. Moreover, the examples given in US '217 do not teach that the non-uniaxial alignment layer 6 is within the liquid crystal material at the cell walls as recited in Claim 1. The Examiner is requested to review the examples set forth in the instant application. See for example page 45, first paragraph of the instant application. Applicants submit that neither US '217 nor any of the cited references teach or suggest that "means for reducing anchoring energy at the surface alignment on one or both cell walls, comprising an oligomer or polymer within the liquid crystal material at the cell walls" as recited by the independent Claims 1, 13, 18, 33 and 44.

Applicants submit in regard to US '217 that:

- (i) the layer (film 6) is not within the liquid crystal material at the cell walls as specifically claimed;
- (ii) there is no specific teaching that the layer (film 6) does in fact result in a lower anchoring energy than the electrode 5 on which the layer is coated;
- (iii) if the substrate 2 has any alignment treatment at all, this comprises the layer 6 itself ("non-uniaxial alignment layer" – which term includes random alignment). This layer is not provided with an oligomer or polymer for reducing anchoring energy; instead it has an optional coating 7 of, eg, a silane coupling agent, which is not at all an oligomer or polymer for reducing anchoring energy;
- (iv) the substrate 1, which does have an alignment treatment, ("alignment control layer 4") is also not provided with an oligomer or polymer within the liquid crystal at the cell wall for reducing anchoring energy;
- (v) even if the layer (film 6) were an oligomer or polymer for reducing anchoring energy, it is only provided on one cell wall, not both, whereas currently pending Claim 1 recites that the oligomer or polymer is within the liquid crystal material at the cell walls (plural).

Applicants further submit that US '217 relates to a liquid crystal device, using a ferroelectric or antiferroelectric liquid crystal. A problem with such devices is that desired halftones can be unstable because of an electric field resulting from localized

ions caused by the spontaneous polarization of the ferroelectric liquid crystal molecules. As explained in column 2, line 53 to column 3, line 12 of US '217 this undesired electric field can cause switching defects. US '217 proposes to reduce this problem by providing first and second substrates having surface potentials having a difference of less than 50 mV. The first substrate has a uniaxial alignment characteristic and the second substrate has a non-uniaxial alignment characteristic. Referring to the examples and Figures 1 and 13 in US '217, this limitation of surface potential difference is achieved by providing a film (6, 96) directly on the electrodes (5, 95) of the second substrate (2, 92). The film (6, 96) has special properties, being selected to control the surface potential and having a preferred volume resistivity in the range 104 – 108 ohm.cm (column 4, line 6). Suitable materials for the film are described in column 12, line 47- column 13, line 6. These materials are inorganic materials such as SiO_x , TiO_x , and ZrO_x , other melttable inorganic oxide, silica and a polymer such as siloxane polymer.

5. Specific examples of coating films (6) are given in column 19, lines 65-67 and column 20, lines 1-4 in US '217. These comprise siloxane (SiO_x) polymer and a film of composite of titanium dioxide, zirconium oxide, silicon oxide etc, with suitable ultrafine particles such as antimony-doped SnO_2 . This coating film (6) comprises the "non-uniaxial alignment layer" on the second substrate. See, for example, column 20, line 52, column 21, lines 36-38, and column 22 lines 34-36.

6. Applicant submit that currently pending Claim 1 is not anticipated by US '217. Moreover, US '217 does not contain any teaching or suggestion to provide an oligomer or polymer within the liquid crystal material at the cell walls, for reducing anchoring energy at the surface alignment on one or both cell walls. Accordingly, currently pending Claim 1 is not obvious in view of US '217. Since the currently independent Claims 13, 18, 33 and 44 have the same limitations as currently pending Claim 1, it is submitted that these Claims are likewise not anticipated by and not obvious in view of US '217.

II. Claim Rejections – 35 U.S.C. § 103

The Examiner rejects Claims 3-59 under 35 U.S.C. § 103(a) beginning on page 3 of the Office Action in view of several references.

1. Rejection of Claim 3 on page 3 of the Office Action

The Examiner rejects Claim 3 in view of US '217 and JP-04-269721) Kazuhiko *et al* (JP '721). JP '721 relates to spacer beads for LCDs. Such beads perform a totally different function from the layer 6 of US '217, namely, separating the cell substrates. The Examiner asserts that it would be obvious to modify US '217 to use an oligomer containing material that would give it a high water wettability for the purpose of lowering surface energy. Firstly, it is not clear that high water wettability would lower surface energy at an interface with a liquid crystal (which is largely immiscible with water). Secondly, the materials from which film 6 are formed are all inorganic oxides with dispersed inorganic oxide particles, selected to achieve a preferred resistivity. It would not have been obvious to one of ordinary skill in the art to replace such a film with an organic polymer such as an acrylate with any expectation of success. Any motivation to combine US '217 with JP '721 is therefore provided by the Applicant's own disclosure, not by the prior art.

2. Claims 4-6 on page 4 of the Office Action

The Examiner rejects Claims 4-6 in view of US '217 and Yamagishi *et al* (US '624). The Examiner asserts that it would have been obvious to one of ordinary skill in the art to modify US '217 in view of US '624 to incorporate an oligomer or polymer for the purpose of affecting surface potential. The Examiner is making an argument coming from a wrong assumption by equating surface potential and anchoring energy as explained above. As has previously been pointed out, US '624 relates to polymer-dispersed LC displays. Polymerisation of a monomer causes phase separation to provide LC pockets dispersed within a polymer matrix. No surface alignment is necessary because alignment is provided by the curved walls of the polymer matrix.

This polymer-dispersed display technology is not compatible with the ferroelectric display technology of US '217, which requires carefully controlled planar alignment of a chiral smectic LC to achieve a state in which the LC layer has a spontaneous polarization. Because the US '217 and US '624 displays work in different and incompatible ways there is no motivation to combine these documents in a reasonable expectation of success. US '217 and US '624 teach away from each other. Any motivation for such a combination is therefore provided by the Applicant's own disclosure, not by the prior art.

3. Rejection of Claim 10 on page 5 of the Office Action

The Examiner rejects Claim 10 in view of US '217 and Onishi *et al* (US '220). The Examiner cites column 2, lines 61-65 of US '220, the only sentence of which reads as follows:

"... Therefore, it is insufficient to pay attention only To [sic] the glass transition temperature Tg of the polymer material To [sic] consider heat resistance that affects the display characteristics ..."

On the basis of this passage, the Examiner asserts that it would have been obvious to one of ordinary skill in the art to modify US '217 in view of US '220 to use a polymer with a glass transition temperature lower than that of the device to ensure a high quality display. The Applicants respectfully traverse the Examiners assertion and submit that to the contrary, US '220 (which again relates to polymer-dispersed liquid crystal displays) teaches the use of polymers having glass transition temperatures above 50°C. This temperature is, of course, is reasonably higher than the operating temperature of most LCDs. Accordingly, the prior art cited and combined by the Examiner clearly does not teach or suggest the Claim limitations of Claim 10 (Tg below the operating temperature range of the device).

4. Rejection of Claims 7-9 and 11-12 on page 6 of the Office Action

The Examiner rejects Claims 7-9 and 11-12 stand rejected in view of a combination of US '217 and Bryan-Brown *et al* (US '264) or Wu *et al* (US '533). The Examiner provides no motivation for one of ordinary skill in the art to combine these

teachings, nor does the Examiner cite any specific passage in any of the citations to support an argument that it would be obvious to arrive at the subject matter of the specified Claims by making the claimed combinations.

5. Rejection of Claim 13 on page 5 of the Office Action

The Examiner rejects Claim 13 on the same grounds as Claim 10. Therefore, Applicants respectfully refer to the previous submission in regard to Claim 10.

6. Rejection of Claims 14-17 on page 6 of the Office Action

The Examiner rejects Claims 14-17 stand rejected in view of a combination of US '217 and Hatano *et al* (US '368). US '368 relates to a display which uses a cholesteric LC distributed within phase-separated polymer domains. Its manufacture is similar to that of other polymer-dispersed LCDs in which the polymer phase-separates out from solution in the LC. As previously discussed, these technologies are not compatible. Moreover, one of ordinary skill in the art would not consider forming the film 6 in US '217 by phase separation from the LC, because this film is formed from an inorganic oxide and contains ultrafine inorganic oxide filler particles to achieve the desired resistivity. Such oxides are not readily soluble in liquid crystals, and particles would be expected to remain in suspension in the liquid crystal.

7. Rejection of Claims 18-32 from page 7 to page 9 of the Office Action

The Examiner rejects Claims 18 in view of Bryan-Brown *et al* (US '459) and US '217. Claim 18 recites that the device is a twisted nematic capable of being switched from a twisted state to a non-twisted state. The examiner asserts that these features are disclosed at column 9 lines 41-43 of US '459. Even if this passage reads "...in both the switched states of a cell the nematic liquid crystal material has no twist across the layer" Applicants submit that *this contrasts with twisted nematic devices where typically the material has a 90° twist*. For cells with a monograting on one cell wall and a bigrading on the other wall there will be an amount of twist in both switched states eg +45° & -45°."

Thus, the cited passage does not describe a twisted nematic capable of being switched from a twisted to a non-twisted state. On the contrary, US '459 relates to bistable nematic displays, in which the LC material is switched between two bistable states. In one device there is no twist across the layer, in another there is always a twist. The optical change depends on the angular aligned direction of the LC molecules, not on a transition from a twisted to an untwisted state. Accordingly, the prior art cited and combined by the Examiner clearly does not teach or suggest the claim limitations of Claim 18. It teaches away from Claim 18. Accordingly dependent Claims 19-32 are not obvious in view of the cited prior art as well.

8. Rejection of Claim 33 on page 9 of the office Action

The Examiner rejects Claim 33 in view of US '459 and Kwon (US '818) and US '217. The teachings of US '217 and US '459 have been discussed above. The Applicant traverse the Examiners rejection. US '818 describes the use of photosensitive polymers as LC alignment layers as an alternative to rubbed polymers. The direction of alignment is controlled by the direction of polarization of UV light. Combining US '818 with US '459 and/or US '217 would not teach or suggest all the claim limitations of Claim 33. At most, one of ordinary skill in the art might attempt to use the materials of US '818 as replacements for the monograting of one embodiment of US '459 or the alignment control layer 4 of US '217. There is no teaching or suggestion in any of the cited art to reduce the anchoring energy in the surface alignment by means of an oligomer or polymer within the liquid crystal at the cell walls. The cited prior references teach away of Claim 33.

9. Rejection of Claims 34-43 from page 10 to page 11 of the Office Action

The Examiner rejects Claims 34-43 by making a combination of four prior art documents against. The Applicant traverse the Examiners rejection and submit that if the independent Claim 33 is not obvious in view of the prior art, the dependent Claims should not be obvious as well. The Examiner's reference to "Wu *et al* (US '017B2)" is not understood by the Applicants. It is assumed that Barberi et al. (US-6,327,017) was meant

to be cited. However, The Examiner does not make any reference to Berberi et al. The Applicants respectfully refer to the submission in our response dated January 30, 2003 in regard to Wu *et al* (US 5,661,533).

10. Rejection of Claim 44 on page 11 of the Office Action

The Examiner rejects Claim 44 in view of US '264 and US '217. The teachings of US' 264 and US' 217 have been previously discussed. Applicants submit that the combination of the teachings of the two references US '264 and US '217 does not teach or suggest all the claim limitations. At most, the combination would result in the use of a grating such as described in US '264 as the "alignment control layer 4" of US '217. For the reasons previously discussed in under I. 4 above, this combination does not teach or suggest all the claim limitations.

11. Rejection of Claims 46-59 from page 11 to page 14 of the Office Action

Applicants submit that independent Claim 44 is not obvious in view of the prior art. Therefore, dependent Claims 46-59 are not obvious as well.

Since the independent Claims 1, 13, 18, 33 and 44 all have the limitation "means for reducing anchoring energy at the surface alignment on one or both cell walls, comprising an oligomer or polymer within the liquid crystal material at the cell walls" it is submitted that non of the cited references teach this limitation. Therefore non of the combined references teach or suggest this claim limitation and therefore non of the combinations teach or suggest all the claim limitations.

Clearly the Examiner has combined the references based on a hindsight reconstruction of the Applicants' claims. Therefore the motivation or suggestion to combine the references is based on the Applicants' own disclosure.

The Applicants submit that the rejection of currently pending independent Claim 1 under 35 U.S.C. 102(e) and currently pending independent Claim, 13, 33 and 44 under

35 and amended independent Claim18 under U.S.C. 103(a) is improper. Applicants respectfully request that the rejection of these Claims on grounds be withdrawn.

If the Examiner maintains the rejection of amended Claims 1, 13, 18, 33 and 44 on grounds, the Applicants respectfully request that the Examiner show how the references teach or suggest every element of the rejected Claims and where the motivation for making the suggested combination can be found in the cited reference. It is believed that independent Claims 1, 13, 18, 33 and 44 are allowable and therefore dependent Claims 3-12, 14-17, 19-32, 34-43 and 46-59 are allowable as well.

This Office Action was made final. Applicants submit that the issuance of a final office action is premature. Currently pending Claim 1 is the originally filed Claim 2 worded in independent form. The Examiner rejected originally filed Claim 2 in the first office action under 35 U.S.C. 103(a) in view of US '264 and US '533 . The Examiner has rejected currently pending Claim 1 (original Claim 2) now under 35 U.S.C 102(e) as being anticipated by US '217. Shifting positions in this manner and making the official action final is improper. It is therefore respectfully requested the Examiner to withdraw the finality of the Office Action.

Accordingly, reconsideration and examination of the present application is respectfully requested.

The application is now in condition for allowance. Allowance of the application at an early date is respectfully requested.

The Applicants reserve the right to seek protection for any unclaimed subject matter either subsequently in the prosecution of the present case or in a divisional or continuation application.

The Commissioner is authorized to charge any additional fees which may be required or credit overpayment to deposit account no. 12-0415. In particular, if this response is not timely filed, then the Commissioner is authorized to treat this response as including a petition to extend the time period pursuant to 37 CFR 1.136 (a) requesting an extension of time of the number of months necessary to make this response timely filed and the petition fee due in connection therewith may be charged to deposit account no. 12-0415.

I hereby certify that this correspondence is being deposited with the United States Post Office with sufficient postage as first class mail in an envelope addressed to Commissioner for Patents

POB 1450, Alexandria, VA 22313-1450 on

September 5, 2003

(Date of Deposit)

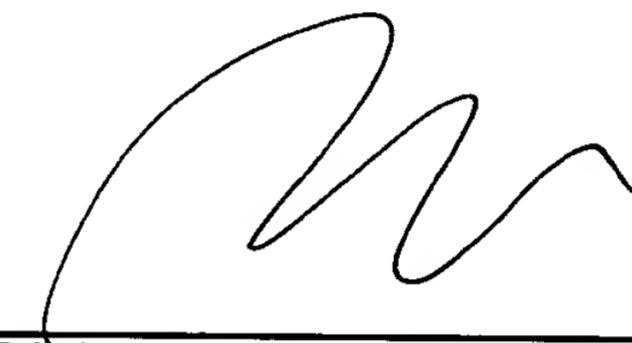
Richard P. Berg

(Name of Person Signing)

(Signature)

September 5, 2003

(Date)



Richard P. Berg
Attorney for Applicants
Reg. No. 28,145
LADAS & PARRY
5670 Wilshire Boulevard, Suite 2100
Los Angeles, California 90036
(323) 934-2300

Respectfully submitted,

Theory and simulation of the nematic anchoring coefficient

DENIS ANDRIENKO^a AND MICHAEL P. ALLEN^b

^aMax-Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

^bDepartment of Physics and Centre for Scientific Computing, University of Warwick, CV4 7AL, United Kingdom



Abstract

Combining molecular simulation, Onsager theory and the elastic description of nematic liquid crystals, we study the dependence of the nematic liquid crystal elastic constants and the zenithal surface anchoring coefficient on the value of the bulk order parameter.

Introduction

The anchoring phenomenon is the tendency of a liquid crystal to orient in a particular direction when in contact with the container walls. The equilibrium director orientation set by the interaction of the liquid crystal with the aligning surface is called an easy orientation axis. The simplest, strong anchoring, assumption is that the director has a fixed orientation at the boundaries along the easy orientation axis. However, it has been discovered that the coupling of the director with the orienting surface can be rather weak. This results in deviation of the surface director from the easy axis in response to small perturbations.

On a phenomenological level, weak anchoring can be described by adding an appropriate surface potential to the free energy of the system. The simplest form of the surface potential has been proposed by Rapini and Papoular [1]

$$f_s = -\frac{1}{2}W(\mathbf{a} \cdot \mathbf{e})^2, \quad (1)$$

where the parameter, W , is termed an anchoring energy.

There have been several attempts to estimate the anchoring coefficient theoretically [2] and by combining molecular simulation with a local density functional approach [3]. The main difficulty here is that one needs to know the direct pair correlation function of the nematic state, which is usually unknown, and must hence be estimated with some uncontrolled approximations or assumptions.

The present work attempts to remedy the situation by combining the elastic description with Onsager theory and Monte Carlo simulation results. We study the dependence of the elastic (K_{33}) and surface anchoring (W) coefficients on the liquid crystal state point, which is defined by the bulk value of the order parameter Q .

Methods

Elastic description

The easiest way to obtain the surface anchoring coefficient W is to create a director deformation far from the surface. Then, measuring the response of the director near the cell surface, or fitting the director profile with a theoretically predicted profile, yields an estimate of the anchoring extrapolation length and ratios of the elastic constants.

Indeed, consider one of the possible geometries suitable for the measurement of the zenithal anchoring strength. Let the director have fixed orientation at the boundary $z = L$. The surface at $z = 0$ is assumed to provide homeotropic anchoring of strength W . In the elastic description, deformations of the director field \mathbf{n} are

$$E(\theta, \delta) = E(\theta_L, \delta) \frac{z + \lambda}{L + \lambda}. \quad (2)$$

Note, that for small angles θ_L and, correspondingly, for small θ , $E(\theta, \delta) = \theta$ and we have linear dependence of the director angle on the z coordinate

$$\delta n_z(z) \approx \theta(z) = \theta_L \frac{z + \lambda}{L + \lambda}. \quad (3)$$

Using eqn (2), one can fit the director profiles $\theta(z)$ with $\lambda = K_{33}/W$ and $\delta = (K_{33} - K_{11})/K_{33}$ as adjustable parameters. To simplify the procedure, it is more appropriate to fit $\theta(z)$ rather than $\theta(z)$.

Onsager approach

The Helmholtz free energy in the Onsager approach is expressed in terms of the single-particle density, $\rho(1)$, where $(1) = (\mathbf{r}_1, \Omega_1)$ represents both position \mathbf{r}_1 and orientation Ω_1 . It has the following form [4]

$$\mathcal{F}[\rho] = \int \rho(1) \{ \ln \rho(1) \Lambda^3 - 1 - \beta \mu + BU(1) \} d(1) - \frac{1}{2} \int f(1, 2) \rho(1) \rho(2) d(1) d(2). \quad (4)$$

Here $\beta = 1/k_B T$, Λ is the de Broglie wavelength, μ is the chemical potential, U is the external potential energy (including the surface potential), and $f(1, 2)$ is the Mayer f -function.

The equilibrium single-particle density that minimizes the free energy (4) is a solution of the following Euler-Lagrange equation

$$\ln \rho(1) \Lambda^3 - \beta \mu + BU(1) - \int f(1, 2) \rho(2) d(2) = 0, \quad (5)$$

which can be obtained from the variation of the functional (4).

Molecular model and simulation methods

We performed Monte Carlo (MC) simulation of a liquid crystal confined between parallel walls, with finite homeotropic anchoring at the walls. The molecules in this study were modeled as hard ellipsoids of revolution of elongation $\epsilon = a/b = 15$.

The slab geometry is defined by two hard parallel confining walls, which cannot be penetrated by the centers of the ellipsoidal molecules.

A sequence of runs was carried out for systems of $N = 2000$ particles using the constant- NVT ensemble, allowing typically 10^4 MC sweeps for equilibration and 4×10^7 sweeps for accumulation of averages. The wall separation was fixed and equal to $L_z \approx 4.93a$.

The same molecular model and interaction of the molecules with the walls was adopted for the Onsager calculations.

Results

Anchoring energy

To obtain the microscopic expression for the extrapolation length λ , we start from the equation for the single-particle density (5). Assume that the solution for a ground state, i.e. for homeotropically aligned liquid crystal in slab geometry, is given by the single-particle density ρ_0 . Consider a small perturbation around the ground state, $\rho = \rho_0 + \delta\rho$. To first order in $\delta\rho$, eqn (5) can be written as

$$\frac{\delta\rho(1)}{\rho_0(1)} = \int f(1, 2) \delta\rho(2) d(2). \quad (6)$$

In the case of slowly-varying director fields we assume that the free energy functional is locally in equilibrium. This is equivalent to the mathematical simplification [5]

$$\rho(\mathbf{r}, \Omega) = \rho_0(\mathbf{r}, \mathbf{n}(\mathbf{r}) \cdot \Omega). \quad (7)$$

In slab geometry, with the z axis normal to the surfaces, the single-particle density ρ_0 depends on the z coordinate only and can be expanded in spherical harmonics. Conducting angular integrations in eqn (6)

$$\begin{aligned} c_{\ell_1}(z_1) \delta n_z(z_1) = 4\pi \sum_{\ell_2=2}^{\infty} \sqrt{\frac{\ell_2(\ell_2+1)}{\ell_1(\ell_1+1)}} \times \\ \int_0^{\infty} A_{\ell_1, \ell_2}(z_2 - z_1) \rho_0(z_2) \delta n_z(z_2) dz_2. \end{aligned} \quad (8)$$

Equation (8) allows one to calculate the director profile (for small director deviations from the ground state) once the single-particle density ρ_0 of the ground state is known.

In the ideal case, often considered in phenomenological approaches [6], the density and order parameter are assumed to be constant in the cell. The anchoring appears only due to the presence of the interface, which breaks translational symmetry. Then the anchoring coefficient is proportional to the first moment of the excluded area coefficient $A_{2,2,1}(z)$

$$\lambda = -\frac{8\pi}{V_{22}} \int_0^{\infty} z A_{2,2,1}(z) dz, \quad (9)$$

and does not depend on the value of density or order parameter, since excluded area, as well as excluded volume, are completely defined by the geometry of the overlapping molecules. This means that in the ideal case of a uniform nematic, the anchoring coefficient $W = K_{33}/\lambda$ has the same dependence on the order parameter as the elastic constant K_{33} .

Onsager theory

Minimization of the grand potential was carried out for the system with an external field applied near the right wall. Profiles of director angle $\theta(z)$ are compared with elastic theory (eqn (2)) in Fig. 1.

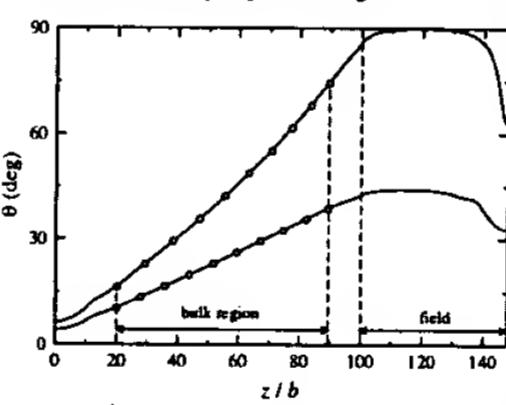


Figure 1 Typical profiles of director angle $\theta(z)$ in the slab geometry. Orienting fields are applied in the region $100 < z/b < 140$ near the right wall, favouring director angles of $\pi/4$ and $\pi/2$ relative to the surface normal. The left wall is unperturbed. Solids lines: Onsager theory. Circles: results of fitting the profiles in the bulk region with the prediction of elastic theory.

The elastic theory has been fitted to the director angle profiles predicted by the Onsager theory using two adjustable parameters. The dependence of the extrapolation length, λ , on the order parameter Q is shown in Fig. 2.

We have also carried out minimization of the grand potential for the system without an external field. As a result, we obtained the single-particle density with a homeotropic distribution of the director in the cell. The dependence of the extrapolation length on the order parameter was then calculated using eqn (8) and is also shown in Fig. 2. The results qualitatively agree with the results of fitting obtained by combining Onsager theory and elastic theory. The extrapolation length tends to grow with increase in the order parameter and has the same order of magnitude.

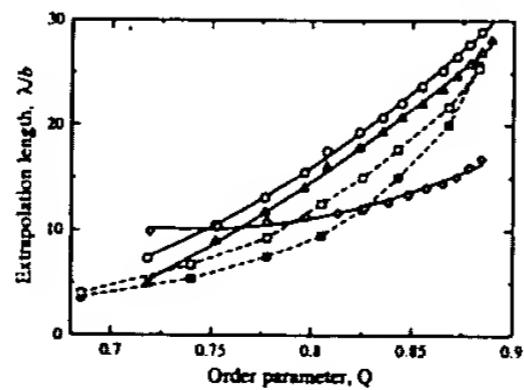


Figure 2 Extrapolation length λ as a function of the order parameter. Circles: Onsager theory in slab geometry, director profiles fitted with elastic theory, for anchoring field with $\alpha = \pi/4$. Triangles: the same, but for $\alpha = \pi/2$. Diamonds: Onsager theory in slab geometry, with no field, extrapolation length calculated using equation (8). Filled squares: Monte Carlo results obtained by measuring director fluctuations. Open squares: Monte Carlo results, with applied field near the right-hand wall.

MC simulation

Simulations were carried out in slab geometry for several values of the number density.

The order tensor fluctuations in reciprocal space were calculated and fitted to the simulation results.

Typical order fluctuation amplitudes together with the corresponding fitting curves are plotted in Fig 3.

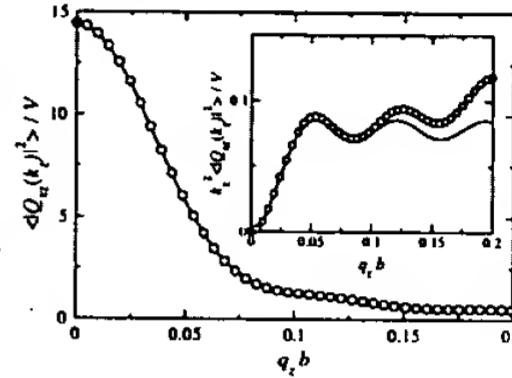


Figure 3 Fluctuations of the director (arbitrary units) as a function of wave-vector (normalized by the molecular minor axis length b). Symbols: Monte Carlo results. Solid lines: elastic theory, fitted to parameters discussed in the text. Inset: fluctuations multiplied by $(k_z b)^2$ to emphasize structure at higher wave numbers.

The dependence of the extrapolation length, λ , on the order parameter Q is shown in Fig 2, together with the results from the Onsager theory. It should be noted that combining the elastic approach with the Onsager calculations does not allow one to determine, separately, L_w and λ . Therefore, the results of the Onsager theory in Fig 2 really represents $\lambda + L_w$, which is one of the possible origins of the systematic difference between the two approaches.

To double check the results obtained by examining the director fluctuation amplitudes, we performed the same type of experiments as in the Onsager slab system. Within a range $7.5b$ of the right-hand wall, a strong coupling field was applied to molecular orientations, $V^{ext} \sim (\mathbf{u}_1 \cdot \mathbf{e}_1)^2$, aligning the molecules near the right wall parallel to it. After the system was equilibrated, the director profile was fitted to the result of the elastic theory, eqn (2). The dependence of the extrapolation length λ on the order parameter Q is also shown in Fig 2. One can see that the agreement between the two methods is quite good.

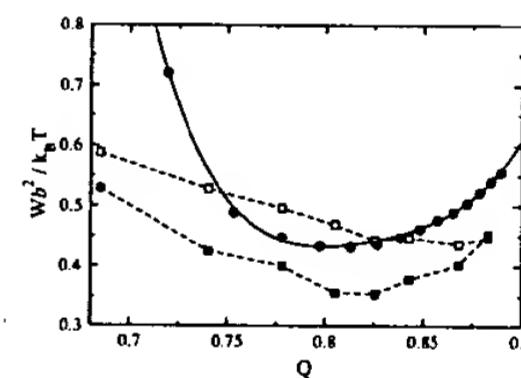


Figure 4 Anchoring energy W as a function of the order parameter. Circles: Onsager theory (with a smooth curve to guide the eye). Open squares: MC results obtained by measuring director fluctuations. Filled squares: MC results, field near the right-hand wall.

Finally, we plot the dependence of the anchoring energy coefficient, $W = K_{33}/\lambda$, which is an intrinsic characteristic of the interface region, in Fig. 4. For Onsager theory, $\lambda(Q)$ is given by the results in slab geometry fitted with the elastic theory (Fig. 2), $K_{33}(Q)$ - by the Poniewierski - Stecki expressions. For MC simulations, we used the elastic constant obtained from the analysis of the director fluctuation amplitudes. All methods predict that the anchoring coefficient is a non-monotonic function of the order parameter, even though the actual variation is small.

Conclusions

We have studied the dependence of the zenithal surface anchoring coefficient on the order parameter of a lyotropic nematic liquid crystal modeled by hard ellipsoids. Several techniques have been used: Onsager theory combined with elastic theory; Monte Carlo simulations fitted to elastic theory; analysis of the director fluctuation amplitudes obtained from Monte Carlo simulations.

A microscopic semi-qualitative expression for the extrapolation length allowed us to conclude that subsurface variations of the single-particle density, mainly defined by the nematic order parameter and density variation, contribute substantially to the anchoring phenomenon. We showed that for an ideal system, in which the single-particle density in the cell is assumed to be uniform, the extrapolation length does not depend on the nematic order parameter. This dependence is therefore associated with the subsurface variations of the single-particle density.

References

- [1] A. Rapini and M. Papoular, *J. de Physique Colloque* 30, C4 (1969).
- [2] B. Tjepkema and D. Sullivan, *J. Chem. Phys.* 88, 6620 (1988).
- [3] J. Stelzer, L. Longa, and H. R. Trebin, *Phys. Rev. E* 55, 7085 (1997).
- [4] R. Evans, in *Fundamentals of Inhomogeneous Fluids*, edited by D. Henderson (Dekker, New York, 1992), chap. 3, pp. 85–175.
- [5] A. M. Sotomayor and P. Tarazona, *Molec. Phys.* 72, 911 (1991).
- [6] H. Yokoyama, *Phys. Rev. E* 55, 2938 (1997).

Acknowledgements

D.A. is grateful to the Alexander von Humboldt foundation.